metry matrices Hs has been determined, the metric symmetry is deduced simply by counting the number of matrices in the group. The greater is the number of matrices, the higher is the symmetry. For example, the numbers of matrices for the seven lattice metric symmetries are: anorthic (triclinic): one; monoclinic: two; orthorhombic: four; rhombohedral: six; tetragonal: eight; hexagonal: twelve; and cubic: twenty-four.

When the symmetry matrices are used to transform an experimentally determined unit cell, metrically similar unit cells are generated. If the lattice symmetry elements correspond to crystallographic symmetry elements, then these metrically similar cells are symmetrically equivalent and the observed metric differences are due to experimental errors. The matrix approach to symmetry provides an ideal way to evaluate the experimental errors simply by averaging the set of tolerance matrices. The resulting "error" matrix [i.e., the averaged tolerance matrix) may be compared directly to the e.s.d.'s for the refined unit cell, or it may be applied to the refined unit cell to calculate an idealized cell reflecting the exact metric symmetry. In either case, the extent to which the refined cell parameters deviate from exact metric symmetry is easily established.

In step **940** the crystal morphology is defined by establishing the crystal size and faces for the primitive cell (basis) defined in step **910**. This step permits absorption corrections to be applied, if necessary, as data is collected in connection with step **950**, to permit the experimental symmetry and conventional cell to be defined.

In step **950**, the crystal symmetry are defined, which entails using the symmetry matrices Hs to generate equivalent intensities (h, k, l)$_{eq}$ from the collected diffraction intensity data (h,k,l) using the equation:

$$\left[\begin{pmatrix} h \\ k \\ l \end{pmatrix}_{eq}\right]_i = Hi \begin{pmatrix} h \\ k \\ l \end{pmatrix}$$

Next, if necessary, absorption corrections are calculated in step **954** from the morphology data derived in step **940**, and the corrections are applied to the equivalent intensities to facilitate comparison thereof. In step **956**, the Laue symmetry is established using the equivalent intensities (h,k,l)$_{eq}$ derived in step **952** (**954**), which the present invention permits to be done without risk of assigning a Laue group of too low a symmetry. In certain cases the intensity measurements will prove that the Laue symmetry is less than that predicted from the metric lattice symmetry. That is, the intensities of all the potentially equivalent (h,k,l)'s are not equal. In these cases, group-subgroup relationships and structural pseudosymmetry can be determined by evaluating the nature of the symmetry matrices in conjunction with the intensity data.

Unlike other methods, the matrix approach of the present invention permits the collection of experimental data and the assignment of the Laue symmetry with respect to any basis. Mistakes in the Laue symmetry are avoided since it is not necessary to do key experimental steps out of order. In the matrix approach, all the data required to assign the Laue symmetry are collected before a conventional cell is determined. In contrast, procedures currently used in diffractometry are based on the risky practice of assuming a conventional cell and symmetry, and then collecting data to verify the assumption. This erroneous strategy may lead to the assignment of a Laue group of too low symmetry.

The next step (**958**) in defining the crystal symmetry is to calculate the nature and directions of the symmetry axes. Since the values of the elements in each symmetry matrix Hs depend upon the kind and orientation of the element with respect to the coordinate system chosen, the symmetry matrices themselves can be analyzed to define both the nature and directions of all symmetry operations of the lattice. The nature of the symmetry axis is found by calculating the trace of the matrix: $tr(H)=H_{11}H_{22}+H_{33}$. The trace of the matrix is invariant under the similarity transformation, i.e., it is independent of the basis chosen. The symmetry axis is an n-fold rotation axis wherein n=1, 2, 3, 4, 6 for tr(H)=3, −1, 0, 1, 2, respectively. Depending on the application, the direction of each axis is given by the solutions q of a linear algebraic equation of the form $(H-1)q=0$, which is the lattice approach, or $((H^{-1})^t-1)q=0$, which is the object approach, where 1 is the identity matrix. The final step **959** in defining the crystal symmetry is to control diffractometer **900** using the symmetry axis data from step **958** to obtain sample orientations for photographs of symmetry in planes of reciprocal space for desired symmetry axes of the primitive cell. As the matrix approach of the present invention enables all symmetry axes to be identified without transformation to standard orientations, all symmetry axes in reciprocal space can be identified once any cell has been determined for an unknown material.

The final step (**960**) in the diffractometer control method of the present invention is to transform the primitive cell to a standard or conventional cell. In a first embodiment of step **960** (FIG. **11**), an idealized cell is calculated (step **962**) by analyzing the cell parameter errors determined in step **930**. The idealized cell is then reduced (step **964**), and then the *International Tables for Crystallography*, Vol. A, published for the International Union of Crystallography by D. Reidel Publishing Comp. (1983), pages 734–735, are searched (step 966) to find a transformation matrix to a conventional cell. This embodiment has the advantage of eliminating all interactions of the cell parameter errors with the reduction calculations. In a second embodiment of step **960**, the nature and directions of the symmetry axes with respect to the original basis for any primitive cell which were experimentally determined in step **958** are also used to obtain a transformation matrix to a standard, conventional, or even a second skewed cell. When choosing a conventional cell, any required metric constraints may be applied separately. A set of conventions used for choosing cell edges based on symmetry, plus additional metric constraints when necessary, are given in the aforementioned *International Tables For Crystallography.*

Two conceptually different approaches may be used to analyze the group of symmetry matrices and to derive a standard cell transformation matrix: the lattice approach and the object approach. Either strategy is ideal for diffractometry. In addition, the choice of directions to be used as cell edges advantageously can be made either through analysis of dependency equations or analysis of determinants. In obtaining a suitable transformation matrix, calculations are carried out with full